Novel η^3-Vinylcarbene Complexes Derived from Ruthenium-Based Olefin Metathesis Catalysts

Supplemental Information

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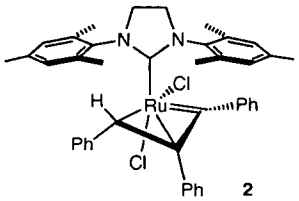
Experimental

General Considerations: All manipulations were performed using a combination of glovebox, high vacuum, and Schlenk techniques under a nitrogen atmosphere, unless otherwise specified. Solvents were dried and degassed by standard procedures. ^{1}H and ^{13}C NMR spectra were measured on a 500 MHz Varian Unity Inova spectrometer. Chemical shifts are reported in ppm relative to $SiMe_4$ ($\delta = 0$) and were referenced internally with respect to the protio solvent impurity ($\delta = 5.32$ for $CDHCl_2$) and the ^{13}C resonances ($\delta = 54.00$ for CD_2Cl_2). ^{19}F spectra were measured on a 300 MHz Varian Mercury spectrometer; chemical shifts were referenced externally to a CCl_3F standard ($\delta = 0$). Coupling constants are in hertz. IR spectra were recorded on a Perkin-Elmer Paragon 1000 spectrophotometer as KBr pellets;

the data are reported in reciprocal centimeters. Elemental analyses were performed by Midwest Microlab, Indianapolis, IN. Diphenylacetylene, 1-phenyl-1-propyne, and 1,4-diphenylbutadiyne were obtained from Aldrich and used as received. $(H_2IMes)(PCy_3)(Cl)_2Ru{=}CHPh$ (**1**) was prepared by an adaptation of a reported synthesis of $(IMes)(PCy_3)(Cl)_2Ru{=}CHPh$ (Wilhelm, T. E.; Grubbs, R. H. **2000**, unpublished results. Modified from: Jafarpour, L.; Nolan, S. P. *Organometallics* **2000**, *19*, 2054-2057). $(H_2IMes)(PCy_3)(Cl)_2Ru{=}CH(p\text{-}C_6H_4F)$ was prepared in an identical manner, starting from $(PCy_3)_2(Cl)_2Ru{=}CH(p\text{-}C_6H_4F)$ (Schwab, P.; Grubbs, R. H.; Ziller, J. W. *J. Am. Chem. Soc.* **1996**, *118*, 100-110). 4,4-dicarbethoxy-2-methyl-1,6-heptadiene was prepared as previously reported (Kirkland, T. A.; Grubbs, R. H. *J. Org. Chem.* **1997**, *62*, 7310-7318).

Synthesis and Characterization of $(H_2IMes)(Cl)_2Ru[\eta^3\text{-}(CHPh)(CPh)(CPh)]$ (2): A Schlenk flask was charged with 0.120 g (0.141 mmol) of $(H_2IMes)(PCy_3)Cl_2Ru{=}CHPh$ (**1**), 0.060 g (0.337 mmol, excess) of diphenylacetylene, and 4 mL of benzene. Under nitrogen, the reaction was heated at 60°C for 5 hours, during which time a dark green precipitate formed. The flask was then opened to air and the reaction mixture filtered through a coarse frit. The isolated green solid was washed with 15 mL hexanes and dried under vacuum. Yield: 0.070 g (66%). NMR assignments were aided with DEPT and COSY experiments. **^{1}H NMR** (499.852 MHz, **25°C**, CD_2Cl_2): δ 1.832 [s, 3H, CH_3], 2.089 [s, 3H, CH_3], 2.240 [s, 3H, CH_3], 2.269 [s, 3H, CH_3], 2.317 [s, 3H, CH_3], 2.552 [s, 3H, CH_3], 3.788 [dt, J = 10 and 12, 1H, NCH_2CH_2N], 4.032 [td, J = 9 and 11, 1H, NCH_2CH_2N], 4.257 [dd, J = 6 and 8, 2H, NCH_2CH_2N], 4.777 [s, 1H, CHPh], 5.803 [s, 1H, m-CH_{Mes}], 6.35 [br s, 1H, Ph], 6.531 [s, 1H, m-CH_{Mes}], 6.667 [s, 1H, m-CH_{Mes}], 6.88-7.03 [multiple peaks, 6H, Ph], 6.978 [s, 1H, m-CH_{Mes}], 7.14 [br s, 2H, Ph], 7.262 [t, J = 7, 1H, p-H of CHPh], 7.46 [br s, 3H, Ph], 7.511 [t, J = 7, 1H, Ph], 9.22 [br s, 1H, o-H of Ru=CPh]. **^{1}H NMR** (499.852 MHz, **-45°C**, CD_2Cl_2): δ 1.772 [s, 3H, CH_3], 1.990 [s, 3H, CH_3], 2.173 [s, 3H, CH_3], 2.217 [s, 3H, CH_3], 2.333 [s, 3H, CH_3], 2.483 [s, 3H, CH_3], 3.740 [dt, J = 11 and 12, 1H, NCH_2CH_2N], 4.003 [td, J = 5 and 11, 1H, NCH_2CH_2N], 4.236 [m, 2H, NCH_2CH_2N], 4.687 [s, 1H, CHPh], 5.635 [s, 1H, m-CH_{Mes}], 6.217 [d, J = 7.5, 1H, Ph], 6.547 [s, 1H, m-CH_{Mes}], 6.703 [s, 1H, m-CH_{Mes}], 6.822 [t, J = 7.5, 1H, Ph], 6.90-6.93 [multiple peaks, 4H, Ph], 6.950 [s, 1H, m-CH_{Mes}], 7.00-7.04 [m, 2H, Ph], 7.164 [d, J = 7.5, 1H, Ph], 7.245 [t, J = 7.5, 1H, Ph], 7.331 [t, J = 7.5, 1H, Ph], 7.440 [t, J = 7.5, 1H, Ph], 7.517 [t, J = 7.5, 1H, Ph], 7.623 [d, J = 7.5, 1H, Ph], 9.169 [d, J = 9, 1H, o-H of Ru=CPh]. **^{1}H NMR** (499.852 MHz, **130°C**, C_6D_5Br): δ 1.93 [br s, 3H, CH_3], 2.11 [br s, 3H, CH_3], 2.32 [br s, 6H, 2 CH_3], 2.58 [br s, 3H, CH_3], 2.81 [br s, 3H, CH_3], 3.77 [br s, 1H, NCH_2CH_2N], 3.90 [br s, 1H, NCH_2CH_2N], 4.17 [br s, 2H, NCH_2CH_2N], 5.032 [s, 1H, CHPh], 6.08 [br s, 1H, m-CH_{Mes}], 6.54 [br s, 1H, m-CH_{Mes}], 6.56 [br s, 1H, m-CH_{Mes}], 6.84-6.87 [multiple peaks, 2H], 6.932 [br t, J = 7, 1H, Ph],



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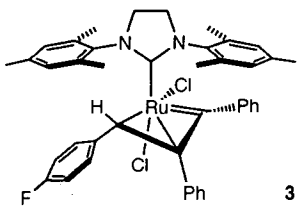
7.025 [br t, J = 7, 2H, Ph], 7.143 [s, 1H], 7.18-7.21 [multiple peaks, 2H, Ph], 7.29-7.38 [multiple peaks, 5H, Ph], 7.49 [s, 1H, Ph], 7.821 [d, J = 7, 1H, Ph], 8.16 [br s, 1H, *o*-H of Ru=CPh]. **$^{13}C\{^1H\}$ NMR** (125.712 MHz, **25°C**, CD_2Cl_2): δ 19.10 [CH_3], 19.27 [CH_3], 19.47 [CH_3], 20.52 [CH_3], 20.02 [CH_3], 21.33 [CH_3], 53.02 [N$\underline{C}H_2\underline{C}H_2$N], 53.64 [N$\underline{C}H_2\underline{C}H_2$N], 67.87 [$\underline{C}$HPhCPhCPh], 91.67 [CHPh$\underline{C}$PhCPh], 127.37 [$CH_{aryl}$], 127.57 [$CH_{aryl}$], 128.26 [$CH_{aryl}$], 128.52 [$CH_{aryl}$], 129.33 [$CH_{aryl}$], 129.47 [$CH_{aryl}$], 130.29 [$CH_{aryl}$], 130.37 [$CH_{aryl}$], 130.90 [$CH_{aryl}$], 132.04 [$C_{aryl}$], 132.12 [br, CH_{aryl}), 134.16 [CH_{aryl}], 134.40 [C_{aryl}], 134.68 [C_{aryl}], 135.26 [C_{aryl}], 136.50 [C_{aryl}], 138.23 [C_{aryl}], 138.95 [C_{aryl}], 139.46 [C_{aryl}], 139.60 [C_{aryl}], 139.68 [C_{aryl}], 141.81 [C_{aryl}], 216.16 [Ru-$\underline{C}N_2(H_2IMes)$], 285.06 [Ru=$\underline{C}$Ph]. **IR:** 3055 (m), 3017 (m), 2953 (m), 2915 (m), 2857 (m), 2730 (w), 2363 (w), 2343 (w), 1609 (m), 1481 (s), 1444 (s), 1426 (s), 1375 (s), 1264 (s), 1181 (m), 1168 (m), 1090 (w), 1075 (m), 1028 (m), 990 (w), 950 (w), 918 (w), 849 (m), 820 (w), 780 (m), 764 (m), 748 (m), 694 (s), 652 (w), 637 (w), 625 (w), 606 (w), 576 (m), 537 (m), 517 (w), 473 (w). **Anal. Calcd. for $C_{42}H_{42}N_2Cl_2Ru$:** C, 67.55%; H, 5.67%; N, 3.75%. Found: C, 67.14%; H, 5.66%; N, 3.56%.

Synthesis and Characterization of $(H_2IMes)(Cl)_2Ru[\eta^3\text{-}(CH(p\text{-}C_6H_4F))(CPh)(CPh)]$ (3): Synthesis analogous to $(H_2IMes)Cl_2Ru[\eta^3\text{-}(CHPh)(CPh)(CPh)]$ (**2**), starting from $(H_2IMes)(PCy_3)Cl_2Ru{=}CH(p\text{-}C_6H_4F)$. **$^1H$ NMR** (499.852 MHz, **25°C**, CD_2Cl_2): δ 1.828 [s, 3H, CH_3], 2.138 [s, 3H, CH_3], 2.237 [s, 3H, CH_3], 2.254 [s, 3H, CH_3], 2.283 [s, 3H, CH_3], 2.558 [s, 3H, CH_3], 3.789 [dt, J = 11 and 12, 1H, NC$\underline{H}_2$C$\underline{H}_2$N], 4.019 [td, J = 7 and 11, 1H, NC$\underline{H}_2$C$\underline{H}_2$N], 4.252 [m, 2H, NC$\underline{H}_2$C$\underline{H}_2$N], 4.719 [s, 1H, C$\underline{H}$(p-C_6H_4F)], 5.835 [s, 1H, *m*-CH_{Mes}], 6.30 [v br s, 1H, Ph], 6.493 [s, 1H, *m*-CH_{Mes}], 6.671 [s, 1H, *m*-CH_{Mes}], 6.850 [br s, 2H], 6.88-6.92 [m, 2H], 6.95-6.97 [m, 4H], 7.021 [tt, J = 1 and 7, 1H], 7.45 [br s, 3H], 7.510 [tt, J = 1 and 7, 1H], 9.20 [br s, 1H, *o*-H of Ru=CPh]. **^1H NMR** (499.852 MHz, **-50°C**, CD_2Cl_2): δ 1.780 [s, 3H, CH_3], 2.050 [s, 3H, CH_3], 2.190 [s, 3H, CH_3], 2.224 [s, 3H, CH_3], 2.295 [s, 3H, CH_3], 2.496 [s, 3H, CH_3], 3.745 [dt, J = 11 and 12, 1H, NC$\underline{H}_2$C$\underline{H}_2$N], 4.001 [td, J = 5 and 11, 1H, NC$\underline{H}_2$C$\underline{H}_2$N], 4.236 [m, 2H, NC$\underline{H}_2$C$\underline{H}_2$N], 4.644 [s, 1H, C$\underline{H}$(p-C_6H_4F)], 5.664 [s, 1H, *m*-CH_{Mes}], 6.238 [d, J = 7, 1H, Ph], 6.533 [s, 1H, *m*-CH_{Mes}], 6.635 [td, J = 2 and 9, 1H, p-C_6H_4F], 6.719 [s, 1H, *m*-CH_{Mes}], 6.837 [t, J = 8, 1H, Ph], 6.91 [br s, 3H, Ph], 6.961 [s, 1H, *m*-CH_{Mes}], 7.052 [m, 3H, Ph], 7.201 [td, J = 2 and 7, 1H, p-C_6H_4F], 7.441 [t, J = 8, 1H, Ph], 7.529 [td, J = 1 and 7, 1H, p-C_6H_4F], 7.608 [td, J = 2 and 7, 1H, p-C_6H_4F], 9.160 [d, J = 8, 1H, *o*-H of Ru=CPh]. **^{19}F NMR** (282.148 MHz, **25°C**, CD_2Cl_2): δ -113.4 (m, p-C_6H_4F).



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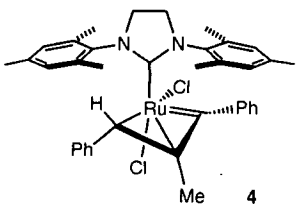
Synthesis and Characterization of $(H_2IMes)(Cl)_2Ru[\eta^3\text{-}(CHPh)(CMe)(CPh)]$ (4): A Schlenk flask was charged with 0.102 g (0.120 mmol) of $(H_2IMes)(PCy_3)Cl_2Ru{=}CHPh$, 0.080 g (0.689 mmol, excess)



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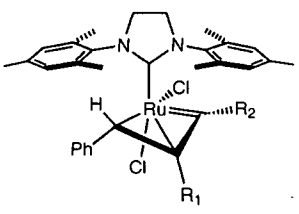
of 1-phenyl-1-propyne, and 4 mL of benzene. Under nitrogen, the reaction was heated at 60°C for 10 hours, during which time an emerald green precipitate formed. The flask was then opened to air and the reaction mixture filtered through a coarse frit. The isolated green solid was washed with 1 mL benzene, 2x10 mL methanol, and 15 mL hexanes, and dried under vacuum. Yield: 0.064 g (78%). **^{1}H NMR** (499.852 MHz, **25°C**, CD_2Cl_2): δ 1.794 [d, J = 0.5, 3H, CMe], 1.872 [s, 3H, CH_3], 2.037 [s, 3H, CH_3], 2.061 [s, 3H, CH_3], 2.227 [s, 3H, CH_3], 2.295 [s, 3H, CH_3], 2.597 [s, 3H, CH_3], 3.782 [dt, J = 10 and 11, 1H, NCH_2CH_2N], 3.940 [td, J = 7 and 11, 1H, NCH_2CH_2N], 4.146 [dt, J = 10 and 11, 1H, NCH_2CH_2N], 4.259 [td, J = 7 and 11, 1H, NCH_2CH_2N], 4.557 [s, 1H, CHPh], 5.974 [s, 1H, m-CH_{Mes}], 6.401 [s, 1H, m-CH_{Mes}], 6.543 [s, 1H, m-CH_{Mes}], 6.975 [s, 1H, m-CH_{Mes}], 7.26-7.30 [multiple peaks, 5H, Ph], 7.344 [tt, J = 1 and 6, 1H, Ph], 7.53-7.55 [m, 2H, Ph], 7.640 [tt, J = 1 and 7, 1H, Ph], 7.90 [br s, 1H, Ph]. **^{1}H NMR** (499.852 MHz, **-70°C**, CD_2Cl_2): δ 1.795 [s, 3H, CMe], 1.808 [s, 3H, CH_3], 1.959 [s, 3H, CH_3], 2.099 [s, 3H, CH_3], 2.158 [s, 3H, CH_3], 2.182 [s, 3H, CH_3], 2.488 [s, 3H, CH_3], 3.719 [dt, J = 11 and 11, 1H, NCH_2CH_2N], 3.916 [td, J = 6 and 11, 1H, NCH_2CH_2N], 4.137 [dt, J = 11 and 11, 1H, NCH_2CH_2N], 4.200 [td, J = 6 and 11, 1H, NCH_2CH_2N], 4.402 [s, 1H, CHPh], 5.739 [s, 1H, m-CH_{Mes}], 6.451 [s, 1H, m-CH_{Mes}], 6.604 [s, 1H, m-CH_{Mes}], 6.902 [d, J = 8, 1H, Ph], 6.959 [s, 1H, m-CH_{Mes}], 7.175 [t, J = 7, 1H, Ph], 7.27-7.35 [multiple peaks, 3H, Ph], 7.396 [t, J = 7, 1H, Ph], 7.535 [br d, 2H, Ph], 7.644 [td, J = 1 and 7, 1H, Ph], 7.498 [d, J = 7, 1H, Ph]. **^{13}C{^{1}H} NMR** (125.712 MHz, **22°C**, CD_2Cl_2): δ 11.49 [CMe], 18.62 [CH_3], 19.17 [CH_3], 19.46 [CH_3], 20.69 [CH_3], 21.07 [CH_3], 21.32 [CH_3], 52.92 [NCH_2CH_2N], 52.98 [NCH_2CH_2N], 69.92 [CHPhCMeCPh], 91.67 [CHPhCMeCPh], 127.60, 128.43, 129.12, 129.54 (br), 129.60, 130.34, 130.36, 130.89, 131.13, 134.18, 134.66, 135.15, 136.54, 138.06, 138.74, 139.28, 139.33, 139.78, 141.67, 214.68 [Ru-$CN_2(H_2IMes)$], 288.142 [Ru=CPh]. **IR:** 3051 (w), 3009 (w), 2947 (w), 2913 (m), 2854 (w), 1623 (m), 1600 (w), 1477 (s), 1459 (m), 1441 (m), 1425 (m), 1400 (m), 1374 (m), 1284 (m), 1265 (s), 1218 (w), 1176 (w), 1166 (w), 1073 (w), 1031 (m), 1012 (w), 984 (w), 849 (m), 803 (w), 756 (m), 692 (m), 632 (w), 575 (w), 559 (w), 497 (w). **Anal. Calcd. for $C_{37}H_{40}N_2Cl_2Ru$:** C, 64.90%; H, 5.89%; N, 4.09%. Found: C, 64.84%; H, 5.89%; N, 3.96%.

Synthesis and Characterization of $(H_2IMes)(Cl)_2Ru[\eta^3$-(CPh)(CC≡CPh)(CHPh)] (5) + Isomer (6):



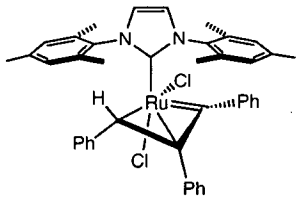
5 R_1 = C≡CPh, R_2 = Ph
6 R_1 = Ph, R_2 = C≡CPh

A Schlenk flask was charged with 0.115 g (0.135 mmol) of $(H_2IMes)(PCy_3)Cl_2Ru$=CHPh, 0.068 g (0.336 mmol, excess) of 1,4-diphenylbutadiyne, and 4 mL of benzene. Under nitrogen, the reaction was heated at 60°C for 12 hours, during which time a dark brown-green precipitate formed. The flask was then opened to air and the reaction

mixture filtered through a coarse frit. The isolated green solid was washed with 15 mL hexanes and dried under vacuum. Yield: 0.057 g (54%). **^{1}H NMR** (499.852 MHz, **25°C**, CD_2Cl_2): δ 1.86 [br s], 2.04-2.40 [multiple peaks, some br], 2.53 [br s], 3.50 [br s], 3.828 [dt, J = 10, 11], 4.01 [br s], 4.24 [br s], 4.64 [br s], 5.85 [br s], 5.90 [br s] 6.54 [br s], 6.72-7.40 [multiple peaks, some br], 7.91 [br s], 8.19 [br s], 9.36 [br s]. **^{1}H NMR** (499.852 MHz, **-30°C**, CD_2Cl_2) diagnostic peaks of the major isomer (~60% of mixture): δ 1.819 [s, 3H, CH_3], 2.069 [s, 3H, CH_3], 2.202 [s, 3H, CH_3], 2.227 [s, 3H, CH_3], 2.259 [s, 3H, CH_3], 2.489 [s, 3H, CH_3], 3.793 [m, 1H, NCH_2CH_2N], 4.015 [m, 1H, NCH_2CH_2N], 4.246 [m, 2H, NCH_2CH_2N], 4.575 [s, 1H, CHPh], 5.727 [s, 1H, *m*-CH_{Mes}], 6.553 [s, 1H, *m*-CH_{Mes}], 6.736 [s, 1H, *m*-CH_{Mes}], 6.956 [s, 1H, *m*-CH_{Mes}]; other peaks δ 1.962 (s), 2.022 (s), 2.089 (s), 2.114 (s), 2.131 (s), 2.138 (s), 2.192 (s), 2.362 (s), 2.573 (s), 3.793 (m), 4.108 (m), 5.891 (s), 6.679 (s), 6.703 (s), 6.763 (s), 6.772 (s), 6.885 (s), 7.009 (s), 7.054 (s), 7.071 (s), 7.481-7.150 (multiple peaks), 7.718-7.652 (multiple peaks), 7.905 (br s), 8.024 (d), 8.90 (v br s). It was not possible to obtain a $^{13}C\{^1H\}$ NMR spectrum because of the poor solubilities of **5** and **6**. **IR:** 3051 (w), 2999 (w), 2958 (w), 2914 (m), 2854 (w), 2195 [w, ν(C≡C)], 1628 (w), 1608 (w), 1592 (w), 1479 (s), 1441 (s), 1427 (s), 1400 (m), 1375 (m), 1280 (s), 1262 (s), 1181 (m), 1130 (w), 1099 (w), 1068 (w), 1028 (m), 989 (w), 912 (w), 883 (w), 850 (m), 812 (w), 759 (s), 725 (w), 688 (s), 652 (w), 637 (w), 576 (m), 530 (m), 512 (w), 474 (w). The product was recrystallized from methylene chloride/hexanes prior to elemental analysis. **Anal. Calcd. for $C_{45}H_{44}Cl_2N_2Ru$:** C, 68.56%; H, 5.49%; N, 3.63%. Found: C, 68.67%; H, 5.72%; N, 3.80%.

Procedure for Polymerization of Diphenylacetylene with 1 and 2: In the glovebox, a glass ampoule was charged with 1.04 g diphenylacetylene and 1 mol % of catalyst **1** or **2**. The ampoule was sealed and immersed in an 80°C oil bath for 20 hrs. The product was washed with 50 mL methylene chloride and dried under high vacuum to yield a soft, pale yellow material (~0.7 g). It was not possible to obtain any other characterization data because of the insolubility of the polymer.

Reaction of (IMes)(PCy$_3$)(Cl)$_2$Ru=CHPh with Diphenylacetylene to generate (IMes)(Cl)$_2$Ru[η^3-(CPh)(CPh)(CHPh)]: A screw-cap Wilmad NMR tube was charged with 0.01 g (0.012 mmol) of (IMes)(PCy$_3$)Cl$_2$Ru=CHPh, 0.01 g (0.056 mmol, excess) of diphenylacetylene, and 0.75 mL of CD_2Cl_2 under nitrogen. The reaction was heated at 60°C for 5 hours, during which time the solution color changed from dark red-brown to dark green. Characteristic **^{1}H NMR** data of the product (499.852 MHz, **25°C**, CD_2Cl_2): δ 1.899 [s, 3H, CH_3], 1.911 [s, 3H, CH_3], 1.987 [s, 3H, CH_3], 2.109 [s, 3H, CH_3], 2.390 [s, 3H, CH_3], 2.416 [s, 3H, CH_3], 5.421 [s, 1H, CPhCPhCHPh],



6.087 [s, 1H, *m*-CH_{Mes}], 6.363 [s, 1H, *m*-CH_{Mes}], 6.546 [s, 1H, *m*-CH_{Mes}], 6.9-7.9 (multiple peaks, CH_{aryl} and NCHCHN).

Crystal Structure Determination of $(H_2IMes)(Cl)_2Ru[\eta^3\text{-}(CHPh)(CPh)(CPh)]$ (2):

Empirical formula	$C_{42}H_{42}Cl_2N_2Ru \bullet 3CH_2Cl_2$
Formula weight	1001.58
Crystallization method	Slow evaporation of a dichloromethane solution
Crystal habit	Lozenge
Crystal size	0.29 x 0.26 x 0.13 mm^3
Crystal color	Opaque green

Data Collection

Preliminary Photos	Rotation
Type of diffractometer	CCD area detector
Wavelength	0.71073 Å MoKα
Data Collection Temperature	98(2) K
θ range for 24446 reflections used in lattice determination	2.24 to 28.59°
Unit cell dimensions	a = 12.3298(7) Å
	b = 17.7113(9) Å β = 100.141(1)°
	c = 21.4653(11) Å
Volume	4614.3(4) $Å^3$
Z	4
Crystal system	Monoclinic
Space group	$P2_1/c$
Density (calculated)	1.442 Mg/m^3
F(000)	2048
Data collection program	Bruker SMART v5.606
θ range for data collection	1.50 to 28.66°
Completeness to θ = 28.66°	94.4 %
Index ranges	$-16 \le h \le 15, -23 \le k \le 22, -28 \le l \le 28$

Data collection scan type	ω scans at 6 ϕ settings
Data reduction program	Bruker SAINT v6.02
Reflections collected	81483
Independent reflections	11204 [R_{int}= 0.1253]
Absorption coefficient	0.837 mm^{-1}
Absorption correction	None
Max. and min. transmission (calculated)	0.8969 and 0.7904

Structure Solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Direct methods
Secondary solution method	Difference Fourier map
Hydrogen placement	Difference Fourier map
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	11204 / 0 / 673
Treatment of hydrogen atoms	Unrestrained except for riding solvent hydrogens
Goodness-of-fit on F^2	2.454
Final R indices [I>2σ(I), 8109 reflections]	R1 = 0.0691, *w*R2 = 0.1195
R indices (all data)	R1 = 0.0964, *w*R2 = 0.1224
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.014
Average shift/error	0.000
Largest diff. peak and hole	2.383 and -1.739 e·$Å^{-3}$

Special Refinement Details

Three molecules of dichloromethane are included in each asymmetric unit as solvent of crystallization. The largest peaks in the final difference Fourier map (four of which are greater than 1 e·$Å^{-3}$) are located near chlorine atoms of the solvent or within 1 Å of the ruthenium.

Refinement of F^2 against all reflections. The weighted R-factor (*w*R) and goodness of fit (S) are based on F^2, conventional R-factors (R) are based on F, with F set to zero for negative F^2. The threshold

expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on all data will be even larger.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Graphics were prepared with the Diamond and SHELXTL programs.

References

Bruker (1999) SMART (v5.606), SAINT (v6.02) and SHELXTL (v5.1). Bruker AXS Inc., Madison, Wisconsin, USA.

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Displacement ellipsoid plot of $(H_2IMes)(Cl)_2Ru[\eta^3\text{-}(CHPh)(CPh)(CPh)]$ (2) with all atom labels:

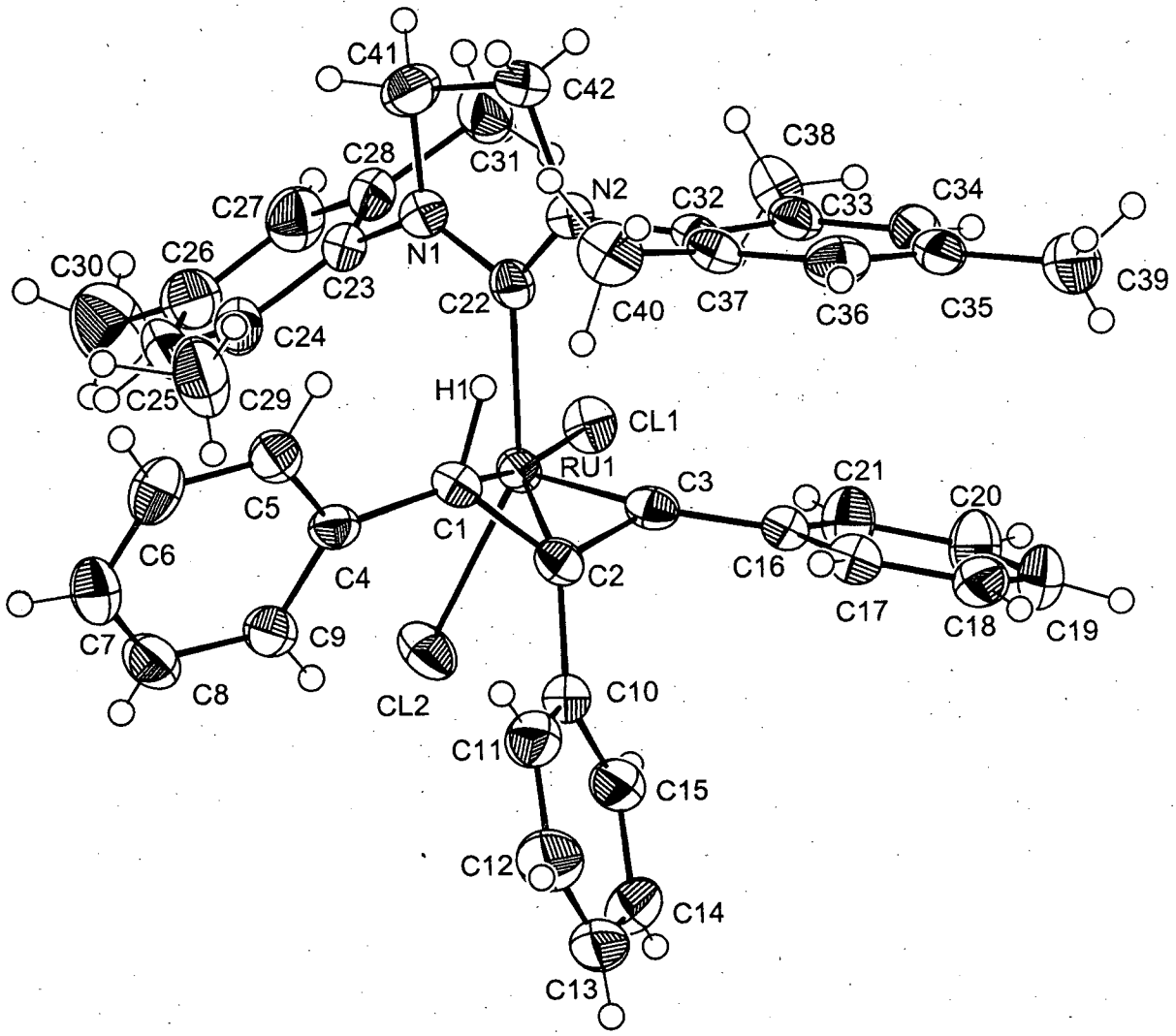

Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for (H_2IMes)(Cl)$_2$Ru[η^3-(CHPh)(CPh)(CPh)] (2). U(eq) is defined as the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U_{eq}
Ru(1)	9249(1)	9044(1)	7067(1)	26(1)
Cl(1)	10869(1)	9491(1)	6739(1)	34(1)
Cl(2)	9967(1)	7815(1)	6996(1)	41(1)
N(2)	8362(3)	10549(2)	7521(2)	28(1)
N(1)	9899(3)	10138(2)	8095(2)	32(1)
C(1)	7596(4)	8789(2)	7436(2)	27(1)
C(2)	7514(3)	8669(2)	6781(2)	27(1)
C(3)	8047(4)	9219(2)	6446(2)	28(1)
C(4)	7425(4)	8212(2)	7907(2)	29(1)
C(5)	6867(4)	8426(3)	8390(2)	36(1)
C(6)	6711(4)	7909(3)	8863(2)	42(1)
C(7)	7128(4)	7201(3)	8862(2)	43(1)
C(8)	7688(5)	6982(3)	8396(2)	41(1)
C(9)	7835(4)	7476(2)	7914(2)	37(1)
C(10)	7062(4)	7958(2)	6441(2)	32(1)
C(11)	6096(5)	7646(3)	6563(2)	41(1)
C(12)	5611(5)	7044(3)	6224(3)	50(2)
C(13)	6090(5)	6730(3)	5753(3)	51(2)
C(14)	7047(6)	7035(3)	5622(2)	50(2)
C(15)	7524(5)	7640(3)	5962(2)	38(1)
C(16)	7794(4)	9487(2)	5796(2)	29(1)
C(17)	6691(4)	9517(2)	5483(2)	34(1)
C(18)	6463(5)	9749(3)	4864(2)	42(1)
C(19)	7283(5)	9942(3)	4540(2)	46(1)
C(20)	8361(5)	9918(3)	4839(2)	48(1)
C(21)	8614(4)	9704(3)	5470(2)	40(1)
C(22)	9154(4)	10020(2)	7564(2)	27(1)
C(23)	10911(4)	9739(2)	8305(2)	31(1)
C(24)	10934(4)	9019(3)	8593(2)	39(1)
C(25)	11957(5)	8692(3)	8792(2)	46(1)
C(26)	12937(5)	9026(3)	8734(2)	47(1)
C(27)	12885(5)	9744(3)	8456(2)	44(1)
C(28)	11906(4)	10096(2)	8236(2)	36(1)
C(29)	9907(6)	8640(4)	8710(3)	61(2)
C(30)	14036(7)	8651(6)	8965(5)	76(2)
C(31)	11890(6)	10849(3)	7916(3)	46(2)
C(32)	7654(4)	10805(2)	6948(2)	27(1)
C(33)	8150(4)	11174(2)	6487(2)	30(1)
C(34)	7459(5)	11449(3)	5959(2)	37(1)
C(35)	6318(4)	11403(2)	5874(2)	37(1)
C(36)	5868(4)	11065(3)	6353(2)	38(1)
C(37)	6512(4)	10772(2)	6899(2)	31(1)
C(38)	9362(4)	11284(3)	6564(3)	41(1)
C(39)	5621(6)	11717(4)	5286(3)	53(2)
C(40)	5961(5)	10466(3)	7415(3)	45(1)
C(41)	9571(5)	10759(3)	8480(2)	42(1)
C(42)	8593(5)	11111(3)	8051(2)	36(1)

C(100)	2995(5)	8305(3)	7162(3)	65(2)
Cl(10)	3649(1)	7496(1)	7505(1)	76(1)
Cl(11)	3928(2)	8992(1)	7023(1)	112(1)
C(101)	9039(6)	3005(3)	9466(3)	72(2)
Cl(12)	10225(2)	2859(1)	10025(1)	94(1)
Cl(13)	8109(2)	2248(1)	9438(1)	102(1)
C(102)	7629(16)	10099(6)	9957(4)	249(9)
Cl(14)	8572(3)	9534(2)	9817(1)	149(1)
Cl(15)	6561(3)	10333(2)	9359(2)	173(1)

Table S2. Bond lengths [Å] and angles [°] for $(H_2IMes)(Cl)_2Ru[\eta^3\text{-}(CHPh)(CPh)(CPh)]$ (2).

Ru(1)-C(3)	1.838(4)	C(15)-H(15)	0.71(4)
Ru(1)-C(22)	2.045(4)	C(16)-C(21)	1.382(7)
Ru(1)-C(2)	2.221(4)	C(16)-C(17)	1.407(6)
Ru(1)-C(1)	2.356(4)	C(17)-C(18)	1.373(6)
Ru(1)-Cl(2)	2.3642(11)	C(17)-H(17)	0.92(5)
Ru(1)-Cl(1)	2.3690(12)	C(18)-C(19)	1.367(7)
N(2)-C(22)	1.345(5)	C(18)-H(18)	0.94(5)
N(2)-C(32)	1.451(5)	C(19)-C(20)	1.371(7)
N(2)-C(42)	1.501(5)	C(19)-H(19)	0.91(4)
N(1)-C(22)	1.347(5)	C(20)-C(21)	1.386(6)
N(1)-C(23)	1.436(6)	C(20)-H(20)	0.96(5)
N(1)-C(41)	1.476(6)	C(21)-H(21)	0.87(5)
C(1)-C(2)	1.409(6)	C(23)-C(28)	1.411(7)
C(1)-C(4)	1.478(5)	C(23)-C(24)	1.415(6)
C(1)-H(1)	1.11(4)	C(24)-C(25)	1.384(7)
C(2)-C(3)	1.437(6)	C(24)-C(29)	1.494(8)
C(2)-C(10)	1.511(6)	C(25)-C(26)	1.370(8)
C(3)-C(16)	1.453(5)	C(25)-H(25)	0.85(4)
C(4)-C(5)	1.395(6)	C(26)-C(27)	1.402(7)
C(4)-C(9)	1.397(6)	C(26)-C(30)	1.513(9)
C(5)-C(6)	1.404(6)	C(27)-C(28)	1.366(7)
C(5)-H(5)	0.96(5)	C(27)-H(27)	0.97(4)
C(6)-C(7)	1.355(7)	C(28)-C(31)	1.500(7)
C(6)-H(6)	0.93(5)	C(29)-H(29A)	0.83(6)
C(7)-C(8)	1.368(7)	C(29)-H(29B)	1.05(5)
C(7)-H(7)	0.85(5)	C(29)-H(29C)	1.06(5)
C(8)-C(9)	1.389(7)	C(30)-H(30A)	1.00(6)
C(8)-H(8)	0.70(5)	C(30)-H(30B)	0.92(8)
C(9)-H(9)	0.97(4)	C(30)-H(30C)	0.80(7)
C(10)-C(11)	1.379(7)	C(31)-H(31A)	0.68(6)
C(10)-C(15)	1.382(7)	C(31)-H(31B)	0.94(4)
C(11)-C(12)	1.368(7)	C(31)-H(31C)	0.83(7)
C(11)-H(11)	0.77(4)	C(32)-C(37)	1.395(6)
C(12)-C(13)	1.373(8)	C(32)-C(33)	1.412(6)
C(12)-H(12)	0.77(5)	C(33)-C(34)	1.381(6)
C(13)-C(14)	1.372(9)	C(33)-C(38)	1.487(7)
C(13)-H(13)	0.88(6)	C(34)-C(35)	1.388(7)
C(14)-C(15)	1.369(7)	C(34)-H(34)	0.84(4)
C(14)-H(14)	0.76(4)	C(35)-C(36)	1.387(7)

C(35)-C(39)	1.503(7)	C(2)-C(1)-H(1)	113.5(19)
C(36)-C(37)	1.395(6)	C(4)-C(1)-H(1)	117(2)
C(36)-H(36)	0.94(5)	Ru(1)-C(1)-H(1)	93(2)
C(37)-C(40)	1.499(7)	C(1)-C(2)-C(3)	116.0(3)
C(38)-H(38A)	0.91(4)	C(1)-C(2)-C(10)	124.2(4)
C(38)-H(38B)	1.02(5)	C(3)-C(2)-C(10)	119.1(4)
C(38)-H(38C)	0.86(5)	C(1)-C(2)-Ru(1)	77.4(2)
C(39)-H(39A)	0.99(7)	C(3)-C(2)-Ru(1)	55.5(2)
C(39)-H(39B)	1.00(6)	C(10)-C(2)-Ru(1)	129.6(3)
C(39)-H(39C)	0.70(5)	C(2)-C(3)-C(16)	131.4(4)
C(40)-H(40A)	0.95(7)	C(2)-C(3)-Ru(1)	84.4(2)
C(40)-H(40B)	1.03(6)	C(16)-C(3)-Ru(1)	139.6(3)
C(40)-H(40C)	1.02(6)	C(5)-C(4)-C(9)	118.0(4)
C(41)-C(42)	1.517(7)	C(5)-C(4)-C(1)	118.0(4)
C(41)-H(41A)	0.99(4)	C(9)-C(4)-C(1)	123.9(4)
C(41)-H(41B)	0.97(5)	C(4)-C(5)-C(6)	120.6(4)
C(42)-H(42A)	0.99(5)	C(4)-C(5)-H(5)	118(3)
C(42)-H(42B)	0.76(4)	C(6)-C(5)-H(5)	122(3)
C(100)-Cl(11)	1.735(6)	C(7)-C(6)-C(5)	120.0(5)
C(100)-Cl(10)	1.741(5)	C(7)-C(6)-H(6)	124(3)
C(100)-H(10A)	0.9900	C(5)-C(6)-H(6)	116(3)
C(100)-H(10B)	0.9900	C(6)-C(7)-C(8)	120.3(5)
C(101)-Cl(12)	1.741(7)	C(6)-C(7)-H(7)	119(4)
C(101)-Cl(13)	1.758(6)	C(8)-C(7)-H(7)	120(4)
C(101)-H(10C)	0.9900	C(7)-C(8)-C(9)	121.0(5)
C(101)-H(10D)	0.9900	C(7)-C(8)-H(8)	122(5)
C(102)-Cl(14)	1.603(13)	C(9)-C(8)-H(8)	117(5)
C(102)-Cl(15)	1.719(14)	C(8)-C(9)-C(4)	120.1(5)
C(102)-H(10E)	0.9900	C(8)-C(9)-H(9)	123(2)
C(102)-H(10F)	0.9900	C(4)-C(9)-H(9)	117(2)
C(3)-Ru(1)-C(22)	97.07(16)	C(11)-C(10)-C(15)	117.4(5)
C(3)-Ru(1)-C(2)	40.09(16)	C(11)-C(10)-C(2)	120.0(4)
C(22)-Ru(1)-C(2)	104.85(16)	C(15)-C(10)-C(2)	122.3(4)
C(3)-Ru(1)-C(1)	69.01(17)	C(12)-C(11)-C(10)	121.5(6)
C(22)-Ru(1)-C(1)	81.62(15)	C(12)-C(11)-H(11)	119(3)
C(2)-Ru(1)-C(1)	35.70(14)	C(10)-C(11)-H(11)	119(3)
C(3)-Ru(1)-Cl(2)	111.80(12)	C(11)-C(12)-C(13)	120.2(6)
C(22)-Ru(1)-Cl(2)	150.25(12)	C(11)-C(12)-H(12)	119(4)
C(2)-Ru(1)-Cl(2)	93.45(10)	C(13)-C(12)-H(12)	120(4)
C(1)-Ru(1)-Cl(2)	101.62(10)	C(14)-C(13)-C(12)	119.2(5)
C(3)-Ru(1)-Cl(1)	109.98(14)	C(14)-C(13)-H(13)	130(4)
C(22)-Ru(1)-Cl(1)	90.07(12)	C(12)-C(13)-H(13)	110(4)
C(2)-Ru(1)-Cl(1)	147.05(11)	C(15)-C(14)-C(13)	120.2(6)
C(1)-Ru(1)-Cl(1)	171.36(10)	C(15)-C(14)-H(14)	112(4)
Cl(2)-Ru(1)-Cl(1)	86.77(4)	C(13)-C(14)-H(14)	127(4)
C(22)-N(2)-C(32)	126.7(3)	C(14)-C(15)-C(10)	121.5(6)
C(22)-N(2)-C(42)	111.8(3)	C(14)-C(15)-H(15)	122(3)
C(32)-N(2)-C(42)	116.1(3)	C(10)-C(15)-H(15)	117(3)
C(22)-N(1)-C(23)	127.9(3)	C(21)-C(16)-C(17)	118.6(4)
C(22)-N(1)-C(41)	112.1(4)	C(21)-C(16)-C(3)	121.6(4)
C(23)-N(1)-C(41)	120.0(3)	C(17)-C(16)-C(3)	119.7(4)
C(2)-C(1)-C(4)	125.7(3)	C(18)-C(17)-C(16)	119.3(5)
C(2)-C(1)-Ru(1)	66.9(2)	C(18)-C(17)-H(17)	116(3)
C(4)-C(1)-Ru(1)	126.7(3)	C(16)-C(17)-H(17)	125(3)

C(19)-C(18)-C(17)	121.6(5)	C(34)-C(33)-C(32)	117.2(4)
C(19)-C(18)-H(18)	123(3)	C(34)-C(33)-C(38)	120.6(4)
C(17)-C(18)-H(18)	115(3)	C(32)-C(33)-C(38)	122.2(4)
C(18)-C(19)-C(20)	119.8(5)	C(33)-C(34)-C(35)	123.5(5)
C(18)-C(19)-H(19)	124(2)	C(33)-C(34)-H(34)	113(3)
C(20)-C(19)-H(19)	116(2)	C(35)-C(34)-H(34)	123(3)
C(19)-C(20)-C(21)	119.9(5)	C(36)-C(35)-C(34)	117.2(4)
C(19)-C(20)-H(20)	119(3)	C(36)-C(35)-C(39)	122.5(5)
C(21)-C(20)-H(20)	121(3)	C(34)-C(35)-C(39)	120.3(5)
C(16)-C(21)-C(20)	120.8(5)	C(35)-C(36)-C(37)	122.7(5)
C(16)-C(21)-H(21)	119(3)	C(35)-C(36)-H(36)	126(3)
C(20)-C(21)-H(21)	120(3)	C(37)-C(36)-H(36)	112(3)
N(2)-C(22)-N(1)	109.2(3)	C(36)-C(37)-C(32)	117.7(4)
N(2)-C(22)-Ru(1)	131.3(3)	C(36)-C(37)-C(40)	119.4(5)
N(1)-C(22)-Ru(1)	118.6(3)	C(32)-C(37)-C(40)	122.9(4)
C(28)-C(23)-C(24)	120.0(4)	C(33)-C(38)-H(38A)	106(3)
C(28)-C(23)-N(1)	118.0(4)	C(33)-C(38)-H(38B)	115(3)
C(24)-C(23)-N(1)	122.0(4)	H(38A)-C(38)-H(38B)	106(4)
C(25)-C(24)-C(23)	117.2(5)	C(33)-C(38)-H(38C)	94(4)
C(25)-C(24)-C(29)	120.9(5)	H(38A)-C(38)-H(38C)	116(5)
C(23)-C(24)-C(29)	121.8(5)	H(38B)-C(38)-H(38C)	119(4)
C(26)-C(25)-C(24)	124.2(5)	C(35)-C(39)-H(39A)	116(4)
C(26)-C(25)-H(25)	125(3)	C(35)-C(39)-H(39B)	115(3)
C(24)-C(25)-H(25)	111(3)	H(39A)-C(39)-H(39B)	99(5)
C(25)-C(26)-C(27)	117.1(5)	C(35)-C(39)-H(39C)	117(5)
C(25)-C(26)-C(30)	122.3(6)	H(39A)-C(39)-H(39C)	101(6)
C(27)-C(26)-C(30)	120.6(6)	H(39B)-C(39)-H(39C)	107(6)
C(28)-C(27)-C(26)	122.2(5)	C(37)-C(40)-H(40A)	112(4)
C(28)-C(27)-H(27)	119(2)	C(37)-C(40)-H(40B)	109(4)
C(26)-C(27)-H(27)	119(2)	H(40A)-C(40)-H(40B)	100(5)
C(27)-C(28)-C(23)	119.4(4)	C(37)-C(40)-H(40C)	109(3)
C(27)-C(28)-C(31)	120.2(5)	H(40A)-C(40)-H(40C)	103(5)
C(23)-C(28)-C(31)	120.4(5)	H(40B)-C(40)-H(40C)	124(4)
C(24)-C(29)-H(29A)	110(5)	N(1)-C(41)-C(42)	103.5(4)
C(24)-C(29)-H(29B)	116(3)	N(1)-C(41)-H(41A)	113(3)
H(29A)-C(29)-H(29B)	116(6)	C(42)-C(41)-H(41A)	115(2)
C(24)-C(29)-H(29C)	105(3)	N(1)-C(41)-H(41B)	112(3)
H(29A)-C(29)-H(29C)	107(5)	C(42)-C(41)-H(41B)	117(3)
H(29B)-C(29)-H(29C)	102(4)	H(41A)-C(41)-H(41B)	97(4)
C(26)-C(30)-H(30A)	103(4)	N(2)-C(42)-C(41)	102.3(4)
C(26)-C(30)-H(30B)	109(5)	N(2)-C(42)-H(42A)	115(2)
H(30A)-C(30)-H(30B)	93(6)	C(41)-C(42)-H(42A)	112(2)
C(26)-C(30)-H(30C)	121(6)	N(2)-C(42)-H(42B)	106(3)
H(30A)-C(30)-H(30C)	103(6)	C(41)-C(42)-H(42B)	117(3)
H(30B)-C(30)-H(30C)	122(8)	H(42A)-C(42)-H(42B)	105(4)
C(28)-C(31)-H(31A)	107(6)	Cl(11)-C(100)-Cl(10)	112.1(3)
C(28)-C(31)-H(31B)	106(3)	Cl(11)-C(100)-H(10A)	109.2
H(31A)-C(31)-H(31B)	139(6)	Cl(10)-C(100)-H(10A)	109.2
C(28)-C(31)-H(31C)	101(4)	Cl(11)-C(100)-H(10B)	109.2
H(31A)-C(31)-H(31C)	99(7)	Cl(10)-C(100)-H(10B)	109.2
H(31B)-C(31)-H(31C)	99(5)	H(10A)-C(100)-H(10B)	107.9
C(37)-C(32)-C(33)	121.5(4)	Cl(12)-C(101)-Cl(13)	111.9(3)
C(37)-C(32)-N(2)	119.9(4)	Cl(12)-C(101)-H(10C)	109.2
C(33)-C(32)-N(2)	118.0(4)	Cl(13)-C(101)-H(10C)	109.2

Cl(12)-C(101)-H(10D)	109.2	Cl(15)-C(102)-H(10E)	107.4
Cl(13)-C(101)-H(10D)	109.2	Cl(14)-C(102)-H(10F)	107.4
H(10C)-C(101)-H(10D)	107.9	Cl(15)-C(102)-H(10F)	107.4
Cl(14)-C(102)-Cl(15)	119.8(6)	H(10E)-C(102)-H(10F)	106.9
Cl(14)-C(102)-H(10E)	107.4		

Table S3. Anisotropic displacement parameters ($Å^2 x\ 10^4$) for $(H_2IMes)(Cl)_2Ru[\eta^3$-(CHPh)(CPh)(CPh)] (2). The anisotropic displacement factor exponent takes the form: $-2\pi^2 [\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Ru(1)	305(2)	226(2)	262(2)	22(2)	67(1)	20(2)
Cl(1)	296(6)	364(6)	356(6)	25(4)	92(5)	5(5)
Cl(2)	450(8)	283(6)	514(7)	64(5)	172(6)	90(5)
N(2)	330(20)	249(18)	259(18)	-15(14)	31(15)	-3(16)
N(1)	380(20)	272(19)	286(19)	-3(15)	0(17)	-15(16)
C(1)	270(30)	230(20)	330(20)	6(17)	77(19)	-2(17)
C(2)	250(20)	230(20)	330(20)	13(17)	49(18)	24(18)
C(3)	290(30)	220(20)	340(20)	-42(16)	103(19)	22(17)
C(4)	320(30)	260(20)	280(20)	-41(17)	45(19)	-50(19)
C(5)	410(30)	340(30)	330(20)	10(20)	90(20)	30(20)
C(6)	390(30)	620(30)	290(20)	10(20)	130(20)	20(30)
C(7)	470(30)	450(30)	380(30)	140(20)	110(20)	-20(20)
C(8)	510(40)	290(30)	460(30)	50(20)	120(30)	-20(30)
C(9)	490(30)	320(30)	330(20)	0(20)	140(20)	-10(20)
C(10)	400(30)	280(20)	280(20)	4(18)	20(20)	0(20)
C(11)	470(30)	400(30)	350(30)	-10(20)	90(30)	-40(20)
C(12)	430(40)	460(30)	570(40)	-10(30)	-10(30)	-160(30)
C(13)	670(40)	340(30)	450(30)	-20(20)	-110(30)	-100(30)
C(14)	720(50)	470(30)	300(30)	-60(20)	60(30)	60(30)
C(15)	430(40)	320(30)	390(30)	10(20)	90(30)	-20(30)
C(16)	350(30)	220(20)	280(20)	0(17)	48(19)	-8(19)
C(17)	370(30)	290(20)	360(30)	-7(19)	60(20)	-10(20)
C(18)	490(40)	320(30)	380(30)	-50(20)	-80(30)	30(20)
C(19)	630(40)	460(30)	280(30)	80(20)	70(30)	40(30)
C(20)	510(40)	590(30)	370(30)	140(20)	160(30)	0(30)
C(21)	330(30)	510(30)	370(30)	80(20)	50(20)	0(20)
C(22)	300(30)	250(20)	270(20)	43(17)	88(18)	-35(18)
C(23)	400(30)	280(20)	230(20)	10(17)	7(19)	0(20)
C(24)	460(30)	380(20)	310(20)	60(20)	0(20)	-30(20)
C(25)	580(40)	290(30)	460(30)	130(20)	-30(30)	40(30)
C(26)	480(40)	440(30)	460(30)	-20(20)	-30(20)	110(30)
C(27)	370(30)	490(30)	420(30)	30(20)	0(20)	-70(30)
C(28)	450(30)	320(20)	270(20)	16(18)	-30(20)	-40(20)
C(29)	590(40)	580(40)	610(40)	270(30)	-70(30)	-110(40)
C(30)	550(50)	740(60)	930(60)	160(50)	-40(40)	170(40)
C(31)	520(40)	370(30)	440(30)	70(30)	-30(30)	-120(30)
C(32)	330(30)	180(20)	300(20)	-18(16)	34(19)	24(17)
C(33)	330(30)	210(20)	370(20)	-30(17)	40(20)	32(18)

C(34)	510(30)	280(30)	340(30)	10(20)	120(20)	0(20)
C(35)	450(30)	240(20)	370(30)	-30(19)	-40(20)	40(20)
C(36)	300(30)	370(30)	460(30)	-100(20)	30(20)	0(20)
C(37)	350(30)	190(20)	380(20)	-17(17)	70(20)	34(18)
C(38)	410(30)	360(30)	460(30)	120(30)	90(30)	40(20)
C(39)	620(50)	410(30)	470(40)	10(30)	-100(30)	80(30)
C(40)	370(30)	460(30)	530(30)	10(30)	130(30)	-10(30)
C(41)	460(30)	410(30)	360(30)	-90(20)	-10(20)	70(20)
C(42)	450(30)	260(30)	370(30)	-40(20)	80(20)	10(20)
C(100)	510(40)	450(30)	940(40)	130(30)	-30(30)	-40(30)
Cl(10)	716(12)	467(8)	1067(13)	237(8)	81(9)	13(7)
Cl(11)	758(14)	768(12)	1890(20)	694(13)	377(14)	111(10)
C(101)	1130(60)	560(40)	550(40)	120(30)	340(40)	20(40)
Cl(12)	1078(17)	1203(15)	611(10)	182(9)	320(10)	-49(12)
Cl(13)	1350(20)	1017(14)	759(12)	-170(10)	379(12)	-331(13)
C(102)	5000(300)	1890(120)	720(70)	120(70)	930(120)	1360(150)
Cl(14)	1350(20)	2120(30)	1031(17)	87(18)	333(16)	-530(20)
Cl(15)	2050(40)	1570(30)	1520(20)	-460(20)	170(20)	370(20)

Table S4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for $(H_2IMes)(Cl)_2Ru[\eta^3$-(CHPh)(CPh)(CPh)] (2).

	x	y	z	U_{iso}
H(1)	7490(30)	9390(20)	7563(16)	25(10)
H(5)	6610(40)	8940(30)	8390(20)	53(14)
H(6)	6340(40)	8090(20)	9180(20)	46(14)
H(7)	7110(40)	6920(30)	9180(20)	59(17)
H(8)	7920(50)	6620(30)	8390(30)	60(20)
H(9)	8240(40)	7340(20)	7580(19)	32(12)
H(11)	5840(30)	7800(20)	6838(17)	12(11)
H(12)	5020(40)	6930(30)	6260(20)	32(15)
H(13)	5660(50)	6380(30)	5550(30)	76(19)
H(14)	7410(40)	6880(20)	5400(20)	25(14)
H(15)	8030(30)	7790(20)	5914(17)	1(11)
H(17)	6090(40)	9400(20)	5670(20)	48(15)
H(18)	5720(40)	9720(20)	4670(20)	43(13)
H(19)	7170(30)	10048(19)	4117(17)	18(10)
H(20)	8920(40)	10110(20)	4620(20)	43(13)
H(21)	9290(40)	9710(20)	5670(20)	43(14)
H(25)	11890(40)	8260(20)	8945(19)	30(12)
H(27)	13570(40)	10000(20)	8419(18)	31(12)
H(29A)	9780(50)	8260(30)	8480(30)	80(20)
H(29B)	9230(40)	9000(30)	8730(20)	44(13)
H(29C)	10090(40)	8440(30)	9180(30)	71(16)
H(30A)	14050(60)	8610(30)	9430(30)	90(20)
H(30B)	14570(70)	9020(40)	9020(30)	120(30)
H(30C)	14150(60)	8230(40)	8860(30)	100(30)
H(31A)	12070(60)	11110(40)	8150(30)	80(30)
H(31B)	11360(40)	10810(20)	7550(20)	35(12)

H(31C)	12450(60)	10820(30)	7760(30)	70(20)
H(34)	7800(40)	11620(20)	5682(19)	31(13)
H(36)	5120(40)	10980(30)	6340(20)	55(15)
H(38A)	9480(30)	11550(20)	6220(20)	33(12)
H(38B)	9810(40)	10800(30)	6560(20)	50(14)
H(38C)	9400(40)	11530(30)	6910(30)	63(19)
H(39A)	5880(60)	12190(40)	5130(30)	110(20)
H(39B)	4860(50)	11880(30)	5340(20)	69(19)
H(39C)	5560(50)	11490(30)	5010(30)	70(20)
H(40A)	5250(60)	10680(30)	7400(30)	80(20)
H(40B)	6350(50)	10680(30)	7840(30)	90(20)
H(40C)	5800(50)	9900(30)	7330(30)	90(20)
H(41A)	10190(40)	11110(20)	8638(19)	35(12)
H(41B)	9450(40)	10590(20)	8890(20)	51(15)
H(42A)	7980(40)	11200(20)	8278(19)	34(13)
H(42B)	8690(30)	11490(20)	7899(17)	12(11)
H(10A)	2520	8168	6757	78
H(10B)	2517	8513	7446	78
H(10C)	9245	3070	9043	87
H(10D)	8674	3475	9569	87
H(10E)	7994	10575	10119	299
H(10F)	7303	9878	10305	299